Scientific Annals of Computer Science vol. 36 (1), 2026, pp. 139–173
doi: 10.47743/SACS.2026.1.139

M-polynomial Based Topological Analysis and Comparative Study of SiC_3 Networks

Shibsankar Das [1,2] and Shahzadi Nargis [3]

Abstract

Topological indices are numerical descriptors used in chemical graph theory to characterize the size, branching and connectivity of molecular structures. These descriptors are significantly correlated with a range of physicochemical characteristics and biological activities of a molecular compound. Recently, the M-polynomial approach has been used to represent molecular structures and calculate degree-based topological indices for various graph structures. This study focuses on determining closed-form expressions of the M-polynomial for three types of silicon-carbon structures: SiC_3-$I[a,b]$, SiC_3-$II[a,b]$ and SiC_3-$III[a,b]$, for arbitrary $a > 1, b \geq 1$. Using the obtained M-polynomial, we calculate nine degree-dependent indices for these silicon-carbide structures. The study also includes visualizations of the computed topological indices and the M-polynomial. Furthermore, we have done a novel comparative analysis among the topological indices for these specific structures. The results obtained in this study provide a mathematical foundation for future researchers in the property prediction of these structures.

Keywords: M-polynomial; SiC_3-$I[a,b]$; SiC_3-$II[a,b]$; SiC_3-$III[a,b]$; Degree-based topological indices.

AMS Mathematics Subject Classification 2020: 05C92, 05C31, 05C09, 05C07.

This work is licensed under the Creative Commons Attribution Licence (CC BY)

[1]Corresponding author

[2]Department of Mathematics, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh, India, Email: shib.cgt@gmail.com, shibsankar@bhu.ac.in

[3]Department of Mathematics, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh, India, Email: snargis04@bhu.ac.in

1 Introduction

Graph theory has applications across numerous science and engineering disciplines including mathematics, computer science, chemistry, and biology. One prominent specialized area is chemical graph theory. As a specialized area within mathematical chemistry, Chemical graph theory (CGT) utilizes graph theory to study and model chemical phenomena, whose ideas have been initially given in [3,16,18,35,36]. It focuses on representing chemical compounds as molecular graphs, where atoms are denoted as vertices and bonds are denoted as edges. This mathematical framework allows for the analysis of chemical properties, molecular structures and reactivity using graph-theoretical concepts. CGT provides a powerful mathematical modeling tools for chemical graphs across various fields, including drug design, material science, environmental chemistry, nanotechnology, chemical engineering, etc.

Let us examine a simple, connected and undirected graph $G = \Lambda$, composed of an edge set $E(\Lambda)$ and a vertex set $V(\Lambda)$. In this graph, vertex degree $u \in V(\Lambda)$, written as d_u, is the count of vertices directly connected to it.

Molecular descriptors are highly important in mathematical chemistry, particularly in QSPR/QSAR studies [4,33]. QSPR focuses on correlating molecular structure with physicochemical properties, while QSAR is concerned with correlating molecular structure with biological activities. An example of a molecular descriptor is a topological descriptor, also known as topological indices, which hold a prominent position.

Topological Index

A topological index is a numerical value that relates to a molecule's physical properties. Some important classes of topological indices are distance-based [2], neighborhood degree sum-based [9], degree-based [12], and eccentricity-based [21] topological indices. The physicochemical characteristics such as temperature of vaporization, melting point, molar volume, boiling point, etc. are all studied by topological indices. A powerful tool in CGT, the M-polynomial has shown promise in deriving and analyzing topological indices, which are critical for understanding molecular structure-property relationships. A single polynomial capable of deriving multiple topological indices is highly desirable. The M-polynomial fulfills this requirement, offering valuable insights into degree-based topological indices through its properties [13].

M-Polynomial

Polynomials serve as a unified framework for computing multiple topological indices simultaneously, eliminating the need to calculate each index separately using its individual definitions. By performing operations such as differentiation, integration or their combination applied to a polynomial representation of structure, the desired topological indices can be derived efficiently.

In the literature, one can find various polynomials, including the matching polynomial [14], Schultz polynomial [17], Hosoya polynomial [20], Tutte polynomial [22], and Zhang-Zhang polynomial [38]. In later research, Deutsch and Klavžar developed the M-polynomial concept in [13], establishing it as a computational framework for evaluating several degree-based topological indices. Researchers have employed the M-polynomial and its associated degree-based indices to investigate various chemical structures. Please refer [8, 11, 12, 29].

Definition 1 ([13]). *The M-polynomial of a graph* Λ *is expressible as*

$$M(\Lambda; x, y) = \sum_{\delta \leq i \leq j \leq \Delta} m_{i,j}(\Lambda)\ x^i y^j$$

for a simple connected undirected graph Λ*, where* $\Delta = \max\{d_u | u \in V(\Lambda)\}$, $\delta = \min\{d_u | u \in V(\Lambda)\}$ *and* $m_{i,j}(\Lambda)(i, j \geq 1)$ *is the cardinality of edges* $u_1u_2 \in E(\Lambda)$ *such that* $d_{u_1} = i$, $d_{u_2} = j$.

As specified in [13], a graph invariant is denoted as $I(\Lambda)$ and can be expressed as

$$I(\Lambda) = \sum_{u_1u_2 \in E(\Lambda)} f(d_{u_1}, d_{u_2}),$$

where the function $f(x, y) \geq 0$ is determined by the degree-based topological index and has the symmetric property $f(x, y) = f(y, x)$. We can rewrite the above definition by grouping the edges with the same set of end-degrees as

$$I(\Lambda) = \sum_{\delta \leq i \leq j \leq \Delta} m_{i,j}(\Lambda) f(i, j).$$

Literature Review

During the year 1972, Zagreb indices were first proposed by Gutman and Trinajstić. [19]. Nikolic et al. later modified the second Zagreb index. In

1975 [35], Milan Randić proposed the Randić index, also termed as a branching index or connectivity index. Amic et al. [1], Bollobás and Erdös [6] independently proposed the general Randić index and the inverse Randić index during 1998. D. Vukičević and M. Gasperov presented the Symmetric division deg index in [37]. In 2003, Caporossi et al. introduced the Harmonic index and the inverse sum (indeg) index [7]. Augmented Zagreb index in 2010 [15] was introduced by Furtula et al. These indices offer a profound analytical framework for molecular branching, stability and reactivity in QSAR and QSPR studies. Due to their strong relationship with the topological indices, and the physicochemical and biological properties of chemical compounds, the investigation of topological indices rapidly increased in recent times. V. R. Kulli introduced a degree-based topological index namely the Nirmala index [23]. The Nirmala indices-based entropy estimates of the silicon-carbide networks [25] were recently examined by V. Kumar and S. Das. An excellent correlation between Revan and Banhatti indices and many physicochemical properties of $SiC_3[a, b]$ was shown in [30]. For the metal-organic networks TM-TCNB, Zhao et al. [39] computed the reverse degree-based topological indices. Zhao and Zahid examined the structure of silicon by Banhatti and Revan indices [40]. Very recently, Banhatti indices like Kepler Banhatti, Modified Kepler Banhatti, reverse Kepler Banhatti and modified reverse Kepler Banhatti indices were proposed by Kulli in [24]. For some silicon-carbide networks, the neighborhood degree sum-based molecular indices were computed and their comparative analysis have been done in [9]. Furthermore, based on the applicability, degeneracy and smoothness on Nirmala and Sombor indices were studied in [26]. For a graph Λ, the mathematical formulas for nine degree-dependent topological indices are listed in Table 1.

Motivation

In the literature, several studies on silicon-carbide (Si_2C_3) type networks exist, such as the neighborhood degree sum-based molecular indices [9], the M-polynomial approach [8], neighborhood degree sum-based entropy measures [28], and degree-based entropy measures [10, 25, 27]. More recently, a QSPR analysis of the Elliptic-type entropy measure of $SiC_3[a, b]$ networks has been studied in [5].

Silicon-carbide plays an important role in providing structural models for understanding the topology, stability and properties of materials. Inspired by the aforementioned studies, the present study addresses a gap in the

Table 1: Formulas for nine degree-dependent topological indices.

Index	**Formula**
First Zagreb Index [32]	$M_1(\Lambda) = \sum_{u_1u_2 \in E(\Lambda)} (d_{u_1} + d_{u_2})$
Second Zagreb Index [32]	$M_2(\Lambda) = \sum_{u_1u_2 \in E(\Lambda)} (d_{u_1} d_{u_2})$
Modified Second Zagreb Index [31]	${}^{m}M_2(\Lambda) = \sum_{u_1u_2 \in E(\Lambda)} \frac{1}{d_{u_1} d_{u_2}}$
General Randić Index [6]	$R_{-1/2}(\Lambda) = \sum_{u_1u_2 \in E(\Lambda)} (d_{u_1} d_{u_2})^{-1/2}$
Inverse Randić Index [1]	$RR_{-1/2}(\Lambda) = \sum_{u_1u_2 \in E(\Lambda)} \frac{1}{(d_{u_1} d_{u_2})^{-1/2}}$
Symmetric Division (Deg) Index [8]	$SDD(\Lambda) = \sum_{u_1u_2 \in E(\Lambda)} \left\{ \frac{\min(d_{u_1}, d_{u_2})}{\max(d_{u_1}, d_{u_2})} + \frac{\max(d_{u_1}, d_{u_2})}{\min(d_{u_1}, d_{u_2})} \right\}$
Harmonic Index [8]	$H(\Lambda) = \sum_{u_1u_2 \in E(\Lambda)} \frac{2}{d_{u_1} + d_{u_2}}$
Inverse Sum (Indeg) Index [8]	$ISI(\Lambda) = \sum_{u_1u_2 \in E(\Lambda)} \frac{d_{u_1} d_{u_2}}{d_{u_1} + d_{u_2}}$
Augmented Zagreb Index [15]	$AZI(\Lambda) = \sum_{u_1u_2 \in E(\Lambda)} \left\{ \frac{d_{u_1} d_{u_2}}{d_{u_1} + d_{u_2} - 2} \right\}^3$

literature. While previous study focused on Si_2C_3 type networks using the M-polynomial approach to those networks [8], we are motivated to investigate $SiC_3[a, b]$ type networks using the same approach.

The primary aim of this study is to compute nine well-known degree-dependent topological indices using the unified framework of the M-polynomial, and we perform a novel comparative analysis of these indices across $SiC_3[a, b]$ type networks, which is not present in the literature. The obtained results will provide a mathematical foundation for future researchers conducting QSPR modeling to evaluate the chemical significance of these networks.

2 Computational Approaches to Silicon-Carbide Networks

A crystalline lattice comprising of carbon and silicon atoms termed as silicon-carbide network, which constitutes the silicon-carbide compound. A type of silicon-carbon network (SiC_3) refers specifically to a silicon-carbide-based network. This type of structure is closely related to silicon-carbide materials [34], which are widely known for their high hardness, thermal stability and chemical resistance. These networks can form various structures, like nanotubes, 2D sheets or polymeric chains, and have potential applications

in electronics, material science and nanotechnology because of their unique combination of mechanical, thermal and electronic properties. This article contains SiC structure with a ratio of $1:3$ called silicon-carbide sheets.

2.1 Silicon-Carbide Network SiC_3-$I[a,b]$

For the silicon-carbide SiC_3-$I[a,b]$ structure, parameter 'a' indicates the number of unit cells connected within each row and 'b' indicates the number of rows connected together, where each row consists of 'a' unit cells. The 2D molecular structure of silicon-carbide SiC_3-$I[a,b]$ is depicted in Figure 1. In this figure, the carbon and silicon atoms are represented by colors red and blue, respectively. Observe from the graph of SiC_3-$I[a,b]$, the cardinality of vertices is $8ab$ and the cardinality of edges is $12ab-2a-3b$.

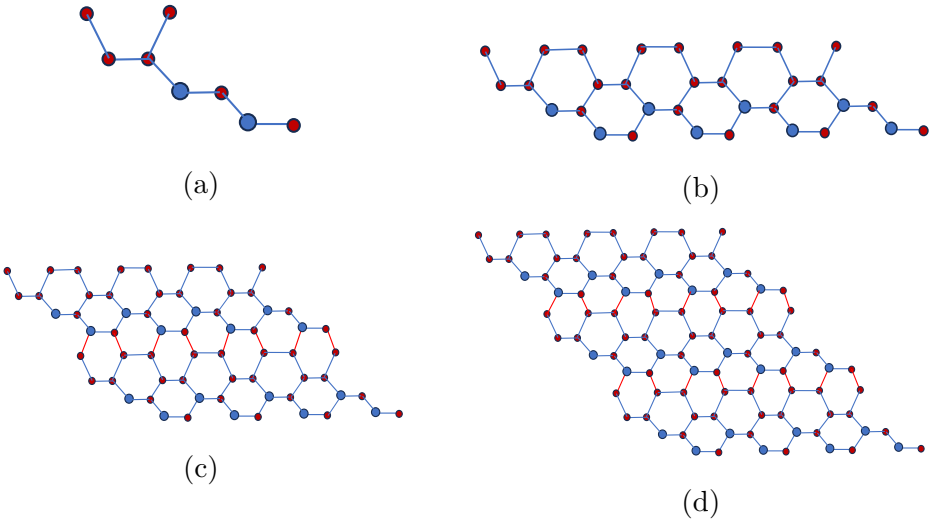


Figure 1: (a) The unit cell of SiC_3-$I[a,b]$, (b) The molecular structure of SiC_3-$I[4,1]$, (c) SiC_3-$I[4,2]$, and (d) SiC_3-$I[4,3]$.

2.1.1 Evaluating the M-polynomial for SiC_3-$I[a,b]$

Theorem 2. *Let SiC_3-$I[a,b]$ be a silicon-carbide network with $a>1, b\geq 1$. Then, the M-polynomial of SiC_3-$I[a,b]$ is given by*

$$\begin{aligned} M(SiC_3\text{-}I[a,b];x,y) =& 2xy^2+xy^3+(2a+2b-3)x^2y^2+(4a+8b-8)x^2y^3 \\ &+(12ab-8b-13a+8)x^3y^3. \end{aligned}$$

Proof. As specified above that for the structure of silicon-carbide SiC_3-$I[a,b]$, we have

$$|V| = 8ab \quad \text{and} \quad |E| = 12ab - 2a - 3b.$$

Now, the values for the five partitions determined by the degree of each edge's terminal vertices are calculated as

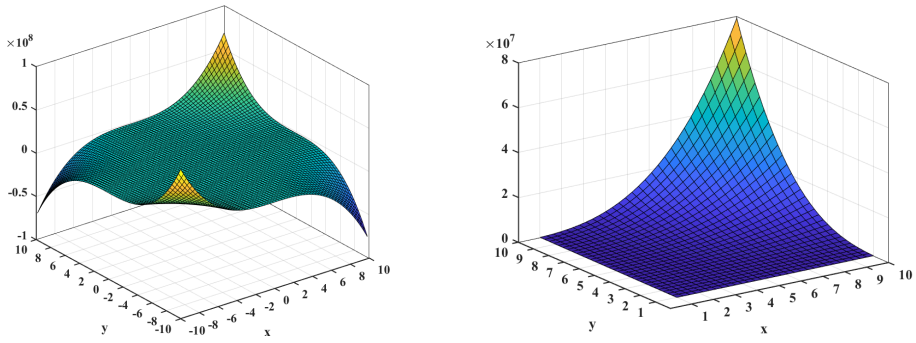
$$\begin{aligned}
E_1 = E_{\{1,2\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}I[a,b]) : d_{u_1} = 1, d_{u_2} = 2\},\\
E_2 = E_{\{1,3\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}I[a,b]) : d_{u_1} = 1, d_{u_2} = 3\},\\
E_3 = E_{\{2,2\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}I[a,b]) : d_{u_1} = 2, d_{u_2} = 2\},\\
E_4 = E_{\{2,3\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}I[a,b]) : d_{u_1} = 2, d_{u_2} = 3\},\\
\text{and} \quad E_5 = E_{\{3,3\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}I[a,b]) : d_{u_1} = 3, d_{u_2} = 3\}.
\end{aligned}$$

Now, we have the generalized formulas for edge-sets of SiC_3-$I[a,b]$ are $|E_1| = 2$, $|E_2| = 1$, $|E_3| = 2a+2b-3$, $|E_4| = 4a+8b-8$, and $|E_5| = 12ab-8b-13a+8$ for $a > 1, b \geq 1$. Therefore by definition, the M-polynomial of SiC_3-$I[a,b]$ is

$$\begin{aligned}
&M(SiC_3\text{-}I[a,b]; x, y)\\
=&\sum_{i\leq j} m_{i,j}x^iy^j, \quad \text{where} \quad i,j \in \{1,2,3\}\\
=&\sum_{1\leq 2} m_{1,2}x^1y^2 + \sum_{1\leq 3} m_{1,3}x^1y^3 + \sum_{2\leq 2} m_{2,2}x^2y^2 + \sum_{2\leq 3} m_{2,3}x^2y^3 + \sum_{3\leq 3} m_{3,3}x^3y^3\\
=&\sum_{u_1u_2\in E_1(SiC_3\text{-}I[a,b])} m_{1,2}x^1y^2 + \sum_{u_1u_2\in E_2(SiC_3\text{-}I[a,b])} m_{1,3}x^1y^3 +\\
&\sum_{u_1u_2\in E_3(SiC_3\text{-}I[a,b])} m_{2,2}x^2y^2 + \sum_{u_1u_2\in E_4(SiC_3\text{-}I[a,b])} m_{2,3}x^2y^3 +\\
&\sum_{u_1u_2\in E_5(SiC_3\text{-}I[a,b])} m_{3,3}x^3y^3\\
=&|E_{\{1,2\}}|x^1y^2 + |E_{\{1,3\}}|x^1y^3 + |E_{\{2,2\}}|x^2y^2 + |E_{\{2,3\}}|x^2y^3 + |E_{\{3,3\}}|x^3y^3\\
=&2xy^2 + xy^3 + (2a+2b-3)x^2y^2 + (4a+8b-8)x^2y^3\\
&+ (12ab-8b-13a+8)x^3y^3.
\end{aligned}$$

□

We used MATLAB R2022a software and Figure 2 presents a visualization of the M-polynomial for the structure SiC_3-$I[4,3]$ within the ranges $1 \leq x, y \leq 10$ and $-10 \leq x, y \leq 10$.



(a) (b)

Figure 2: Plotting M-polynomial of SiC_3-$I[4,3]$: range of (a) $-10 \leq x, y \leq 10$ and range of (b) $1 \leq x, y \leq 10$.

The derivation formulas applied to the M-polynomial, where $f(x,y)$ is a function determined by the mathematical formulation of the degree-based topological index are given as

- For First Zagreb Index:

$$M_1(\Lambda) = (D_x + D_y)(M(\Lambda; x, y))|_{x=y=1}; \text{ where } f(x,y) = x + y.$$

- For Second Zagreb Index:

$$M_2(\Lambda) = (D_x D_y)(M(\Lambda; x, y))|_{x=y=1}; \text{ where } f(x,y) = xy.$$

- For Modified Second Zagreb Index:

$${}^{m}M_2(\Lambda) = (S_x S_y)(M(\Lambda; x, y))|_{x=y=1}; \text{ where } f(x,y) = \frac{1}{xy}.$$

- For General Randić Index:

$$R_\alpha(\Lambda) = (D_x^\alpha D_y^\alpha)(M(\Lambda; x, y))|_{x=y=1}; \text{ where } f(x,y) = (xy)^\alpha.$$

- For Inverse Randić Index:

$$RR_\alpha(\Lambda) = (S_x^\alpha S_y^\alpha)(M(\Lambda; x, y))|_{x=y=1}; \text{ where } f(x,y) = \frac{1}{(xy)^\alpha}.$$

- For Symmetric Division (Deg) Index:

$$SDD(\Lambda) = (D_xS_y+D_yS_x)(M(\Lambda;x,y))|_{x=y=1};\ \text{where } f(x,y) = \frac{x^2+y^2}{xy}.$$

- For Harmonic Index:

$$H(\Lambda) = 2S_xJ(M(\Lambda;x,y))|_{x=1};\ \text{where } f(x,y) = \frac{2}{x+y}.$$

- For Inverse Sum (Indeg) Index:

$$ISI(\Lambda) = S_xJD_xD_y(M(\Lambda;x,y))|_{x=1};\ \text{where } f(x,y) = \frac{xy}{x+y}.$$

- For Augmented Zagreb Index:

$$AZI(\Lambda) = S_x^3Q_{-2}JD_x^3D_y^3(M(\Lambda;x,y))|_{x=1};\ \text{where } f(x,y) = \Big(\frac{xy}{x+y-2}\Big)^3.$$

In Table 2, we tabulate the list of operators which are used in the derivation formulas for the M-polynomial.

Table 2: List of operators.

$D_x = x\frac{\partial(q(x,y))}{\partial x}$,	$D_y = y\frac{\partial(q(x,y))}{\partial y}$,
$S_x = \int_0^x \frac{q(t,y)}{t}dt$,	$S_y = \int_0^y \frac{q(x,t)}{t}dt$,
$Q_\alpha(q(x,y)) = x^\alpha q(x,y),\ \alpha \neq 0.$,	$J(q(x,y)) = q(x,x)$

Theorem 3. *Let SiC_3-$I[a,b]$ be a silicon-carbide network. Then, the degree-based topological indices are given as*

(i) $M_1(SiC_3\text{-}I[a,b]) = 72ab - 50a + 6$,

(ii) $M_2(SiC_3\text{-}I[a,b]) = 108ab - 85a - 16b + 19$,

(iii) ${}^mM_2(SiC_3\text{-}I[a,b]) = \frac{4}{3}ab - \frac{5}{18}a + \frac{17}{18}b + \frac{5}{36}$,

(iv) $R_\alpha(SiC_3\text{-}I[a,b]) = 2^{2\alpha} + 3^\alpha + 2^{2\alpha}(2a+2b-3) + 2^\alpha 3^\alpha(4a+8b-8) + 3^{2\alpha}(12ab-8b-13a+8)$,

(v) $RR_\alpha(SiC_3\text{-}I[a,b]) = 1 + \frac{1}{3^\alpha} + \frac{1}{2^{2\alpha}}(2a+2b-3) + \frac{1}{2^\alpha 3^\alpha}(4a+8b-8) + \frac{1}{3^{2\alpha}}(12ab-8b-13a+8)$,

(vi) $SDD(SiC_3\text{-}I[a,b]) = 24ab - \frac{40}{3}a + \frac{13}{3}b + 1$,

(vii) $H(SiC_3\text{-}I[a,b]) = 4ab - \frac{26}{15}a + \frac{23}{15}b - \frac{1}{5}$,

(viii) $ISI(SiC_3\text{-}I[a,b]) = 18ab - \frac{127}{10}a - \frac{2}{5}b + \frac{89}{60}$,

(ix) $AZI(SiC_3\text{-}I[a,b]) = \frac{2187}{16}ab - \frac{6405}{64}a - \frac{89}{8}b + \frac{564}{8}$.

Proof. Based on the Theorem 2, we have the M-polynomial for $SiC_3\text{-}I[a,b]$ as

$$\begin{aligned} M(SiC_3\text{-}I[a,b];x,y) =& 2xy^2 + xy^3 + (2a+2b-3)x^2y^2 + (4a+8b-8)x^2y^3 \\ &+ (12ab - 8b - 13a + 8)x^3y^3. \end{aligned}$$

We denote $q(x,y) = M(SiC_3\text{-}I[a,b];x,y)$ for notational convenience. Let us now compute the following terms which will be used for determining the topological indices.

- $D_x(q(x,y)) = 2xy^2 + xy^3 + 2(2a+2b-3)x^2y^2 + 2(4a+8b-8)x^2y^3 + 3(12ab-8b-13a+8)x^3y^3$,
- $D_y(q(x,y)) = 4xy^2 + 3xy^3 + 2(2a+2b-3)x^2y^2 + 3(4a+8b-8)x^2y^3 + 3(12ab-8b-13a+8)x^3y^3$,
- $D_yD_x(q(x,y)) = 4xy^2 + 3xy^3 + 4(2a+2b-3)x^2y^2 + 6(4a+8b-8)x^2y^3 + 9(12ab-8b-13a+8)x^3y^3$,
- $S_x(q(x,y)) = 2xy^2 + xy^3 + \frac{1}{2}(2a+2b-3)x^2y^2 + \frac{1}{2}(4a+8b-8)x^2y^3 + \frac{1}{3}(12ab-8b-13a+8)x^3y^3$,
- $S_y(q(x,y)) = xy^2 + \frac{1}{3}xy^3 + \frac{1}{2}(2a+2b-3)x^2y^2 + \frac{1}{3}(4a+8b-8)x^2y^3 + \frac{1}{3}(12ab-8b-13a+8)x^3y^3$,
- $S_xS_y(q(x,y)) = xy^2 + \frac{1}{3}xy^3 + \frac{1}{4}(2a+2b-3)x^2y^2 + \frac{1}{6}(4a+8b-8)x^2y^3 + \frac{1}{9}(12ab-8b-13a+8)x^3y^3$,
- $D_x^{\alpha}D_y^{\alpha}(q(x,y)) = 2^{2\alpha}xy^2 + 3^{\alpha}xy^3 + 2^{2\alpha}(2a+2b-3)x^2y^2 + 2^{\alpha}3^{\alpha}(4a+8b-8)x^2y^3 + 3^{2\alpha}(12ab-8b-13a+8)x^3y^3$,
- $D_xS_y(q(x,y)) = xy^2 + \frac{1}{3}xy^3 + (2a+2b-3)x^2y^2 + \frac{2}{3}(4a+8b-8)x^2y^3 + (12ab-8b-13a+8)x^3y^3$,
- $D_yS_x(q(x,y)) = 4xy^2 + 3xy^3 + (2a+2b-3)x^2y^2 + \frac{3}{2}(4a+8b-8)x^2y^3 + (12ab-8b-13a+8)x^3y^3$,

- $S_x^{\alpha}S_y^{\alpha}(q(x,y)) = xy^2 + \frac{1}{3^{\alpha}}xy^3 + \frac{1}{2^{2\alpha}}(2a+2b-3)x^2y^2 + \frac{1}{2^{\alpha}3^{\alpha}}(4a+8b-8))x^2y^3 + \frac{1}{3^{2\alpha}}(12ab-8b-13a+8)x^3y^3$,

- $S_xJ(q(x,y)) = \frac{2}{3}x^3 + \frac{1}{4}(-2+2a+2b)x^4 + \frac{1}{5}(4a+8b-8)x^5 + \frac{1}{6}(12ab-8b-13a+8)x^6$,

- $S_xJD_xD_y(q(x,y)) = \frac{9}{6}(12ab-8b-13a+8)x^6 + \frac{6}{5}(4a+8b-8)x^5 + (2a+2b-3)x^4 + \frac{3}{4}x^4 + \frac{4}{3}x^3$,

- $S_x^3Q_{-2}JD_x^3D_y^3(q(x,y)) = 2^6x + \frac{3^3}{2^3}x^2 + 2^3(2a+2b-3)x^2 + 2^3(4a+8b-8)x^3 + \frac{3^6}{4^3}(12ab-8b-13a+8)x^4$.

Hence, using the derivation formulas of SiC_3-$I[a,b]$ network, the nine degree-dependent topological indices are given as

(i) $M_1(SiC_3\text{-}I[a,b]) = (D_x+D_y)(q(x,y))|_{x=y=1} = 72ab-50a+6$,

(ii) $M_2(SiC_3\text{-}I[a,b]) = (D_xD_y)(q(x,y))|_{x=y=1} = 108ab-85a-16b+19$,

(iii) ${}^mM_2(SiC_3\text{-}I[a,b]) = (S_xS_y)(q(x,y))|_{x=y=1} = \frac{4}{3}ab - \frac{5}{18}a + \frac{17}{18}b + \frac{5}{36}$,

(iv) $R_{\alpha}(SiC_3\text{-}I[a,b]) = (D_x^{\alpha}D_y^{\alpha})(q(x,y))|_{x=y=1} = 2^{2\alpha} + 3^{\alpha} + 2^{2\alpha}(2a+2b-3) + 2^{\alpha}3^{\alpha}(4a+8b-8) + 3^{2\alpha}(12ab-8b-13a+8)$,

(v) $RR_{\alpha}(SiC_3\text{-}I[a,b]) = (S_x^{\alpha}S_y^{\alpha})(q(x,y))|_{x=y=1} = 1 + \frac{1}{3^{\alpha}} + \frac{1}{2^{2\alpha}}(2a+2b-3) + \frac{1}{2^{\alpha}3^{\alpha}}(4a+8b-8) + \frac{1}{3^{2\alpha}}(12ab-8b-13a+8)$,

(vi) $SDD(SiC_3\text{-}I[a,b]) = (D_xS_y+D_yS_x)(q(x,y))|_{x=y=1} = 24ab - \frac{40}{3}a + \frac{16}{3}b + 1$,

(vii) $H(SiC_3\text{-}I[a,b]) = 2S_xJ(q(x,y))|_{x=1} = 4ab - \frac{26}{15}a + \frac{23}{15}b - \frac{1}{5}$,

(viii) $ISI(SiC_3\text{-}I[a,b]) = S_xJD_xD_y(q(x,y))|_{x=1} = 18ab - \frac{127}{10}a - \frac{2}{5}b + \frac{89}{60}$,

(ix) $AZI(SiC_3\text{-}I[a,b]) = S_x^3Q_{-2}JD_x^3D_y^3(q(x,y))|_{x=1} = \frac{2187}{16}ab - \frac{6405}{64}a - \frac{89}{8}b + \frac{564}{8}$.

□

Table 3: Computation of nine topological indices of SiC_3-$I[a,b]$ by deriving the M-polynomial for various values of a and b.

Sl.	$[a,b]$	$[2,1]$	$[2,2]$	$[2,3]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
	M-polynomial / Topological Index	$2xy^2 + xy^3 + 3x^2y^2 + 8x^2y^3 - 2x^3y^3$	$2xy^2 + xy^3 + 5x^2y^2 + 16x^2y^3 + 14x^3y^3$	$2xy^2 + xy^3 + 7x^2y^2 + 24x^2y^3 + 25x^3y^3$	$2xy^2 + xy^3 + 5x^2y^2 + 12x^2y^3 - 3x^3y^3$	$2xy^2 + xy^3 + 7x^2y^2 + 20x^2y^3 + 25x^3y^3$	$2xy^2 + xy^3 + 9x^2y^2 + 28x^2y^3 + 53x^3y^3$	$2xy^2 + xy^3 + 7x^2y^2 + 16x^2y^3 - 4x^3y^3$	$2xy^2 + xy^3 + 9x^2y^2 + 24x^2y^3 + 36x^3y^3$	$2xy^2 + xy^3 + 11x^2y^2 + 32x^2y^3 + 76x^3y^3$
1.	First Zagreb Index	50	194	338	72	288	504	94	382	670
2.	Second Zagreb Index	49	249	449	72	380	688	95	511	927
3.	Modified Second Zagreb Index	3.1944	6.8056	10.4167	4.2500	9.1944	14.1389	5.3056	11.5833	17.8611
4.	General Randić Index ($\alpha = -1/2$)	5.1767	14.7760	24.3753	7.4763	21.0756	34.6750	9.7760	27.3753	44.9746
5.	Inverse Randić Index ($\alpha = -1/2$)	22.3280	93.9239	165.5198	33.1259	140.7218	248.3178	43.9239	187.5198	331.1157
6.	Symmetric Division (Deg) Index	27.6667	81.0000	134.3333	38.3333	115.6667	193.0000	49.0000	150.3333	251.6667
7.	Harmonic Index	5.8667	15.4000	24.9333	8.1333	21.6667	35.2000	10.4000	27.9333	45.4667
8.	Inverse Sum (Indeg) Index	11.6833	47.2833	82.8833	16.9833	70.5833	124.1833	22.2833	93.8833	165.4833
9.	Augmented Zagreb Index	132.5938	394.8438	657.0938	169.2031	568.1406	967.0781	205.8125	741.4375	1277.0625

2.1.2 Visualizing Topological Indices of SiC_3-$I[a,b]$

Table 3 represents the M-polynomial and the associated indices for different parameters a and b in the SiC_3-$I[a,b]$ structure. To analyze the behavior of the M-polynomial and associated topological indices, we examine parameter values ranging from $a = 2$ to $a = 4$ and $b = 1$ to $b = 3$. Figure 3 displays the graphical representation of nine topological indices over the ranges $2 \leq a \leq 100$ and $1 \leq b \leq 100$ using MATLAB R2022a software. The results demonstrate that all topological indices exhibit increasing values with simultaneous increase of parameters a and b.

2.2 Silicon-Carbide Network SiC_3-$II[a,b]$

It is observed that the cardinality of vertices is $8ab$ and the cardinality of edges is $12ab - 2a - 2b$ in silicon-carbide SiC_3-$II[a,b]$ structure. Figure 4 shows the 2D molecular graph of SiC_3-$II[a,b]$.

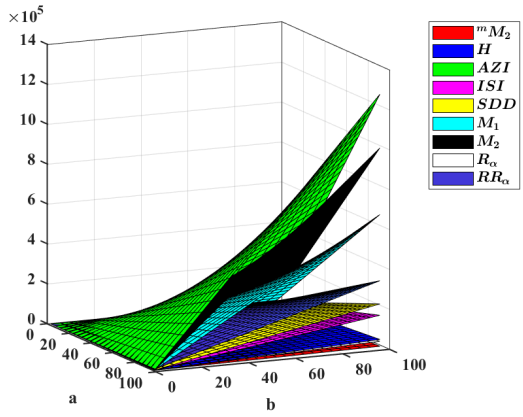


Figure 3: Plotting different parameters a and b ($2 \leq a \leq 100$ and $1 \leq b \leq 100$) of SiC_3-$I[a, b]$ for all nine indices.

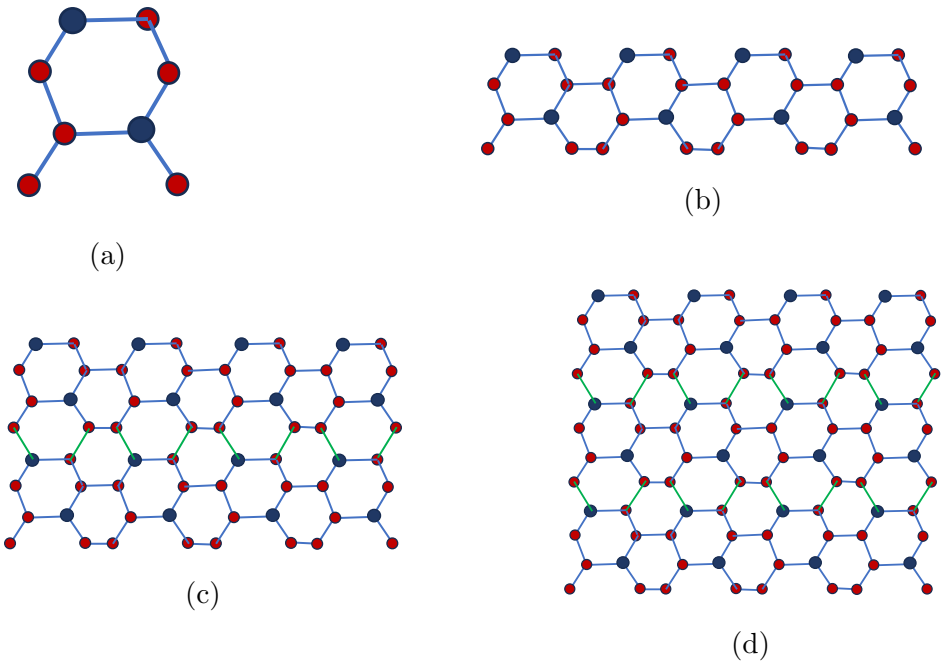


Figure 4: (a) The unit cell of SiC_3-$II[a, b]$, (b) The molecular structure of SiC_3-$II[4, 1]$, (c) SiC_3-$II[4, 2]$, and (d) SiC_3-$II[4, 3]$.

2.2.1 Evaluating the M-polynomial for SiC_3-$II[a, b]$

Theorem 4. *Let SiC_3-$II[a, b]$ be a silicon-carbide network with $a > 1, b \geq 1$. Then, the M-polynomial of SiC_3-$II[a, b]$ is given by*

$$\begin{aligned} M(SiC_3\text{-}II[a,b];x,y) =& 2xy^3 + (2a+1)x^2y^2 + (4a+8b-10)x^2y^3 \\ &+ (12ab-8a-10b+7)x^3y^3. \end{aligned}$$

Proof. As specified above for the structure of SiC_3-$II[a, b]$, we have

$$|V| = 8ab \quad \text{and} \quad |E| = 12ab - 2a - 2b.$$

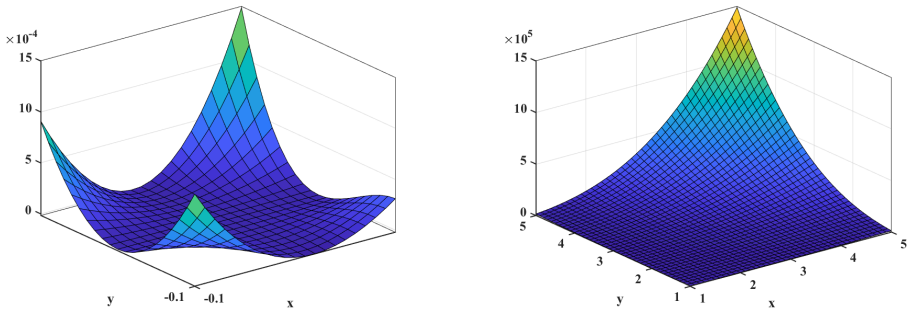
Now, the values for the four partitions determined by the degree of each edge's terminal vertices are calculated as

$$\begin{aligned} E_1 = E_{\{1,3\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}II[a,b]) : d_{u_1} = 1, d_{u_2} = 3\}, \\ E_2 = E_{\{2,2\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}II[a,b]) : d_{u_1} = 2, d_{u_2} = 2\}, \\ E_3 = E_{\{2,3\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}II[a,b]) : d_{u_1} = 2, d_{u_2} = 3\}, \\ \text{and} \quad E_4 = E_{\{3,3\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}II[a,b]) : d_{u_1} = 3, d_{u_2} = 3\}. \end{aligned}$$

Now, we have $|E_1| = 2$, $|E_2| = 2a + 1$, $|E_3| = 4a + 8b - 10$ and $|E_4| = 12ab - 8a - 10b + 7$ for $a > 1, b \geq 1$. Therefore by definition, the M-polynomial of SiC_3-$II[a, b]$ is

$$\begin{aligned} &M(SiC_3\text{-}II[a,b];x,y) \\ &= \sum_{i\leq j} m_{i,j}x^iy^j, \quad \text{where} \quad i,j \in \{1,2,3\} \\ &= \sum_{1\leq 3} m_{1,3}x^1y^3 + \sum_{2\leq 2} m_{2,2}x^2y^2 + \sum_{2\leq 3} m_{2,3}x^2y^3 + \sum_{3\leq 3} m_{3,3}x^3y^3 \\ &= \sum_{u_1u_2\in E_1(SiC_3\text{-}II[a,b])} m_{1,3}x^1y^3 + \sum_{u_1u_2\in E_2(SiC_3\text{-}II[a,b])} m_{2,2}x^2y^2 + \\ &\quad \sum_{u_1u_2\in E_3(SiC_3\text{-}II[a,b])} m_{2,3}x^2y^3 + \sum_{u_1u_2\in E_4(SiC_3\text{-}II[a,b])} m_{3,3}x^3y^3 \\ &= |E_{\{1,3\}}|x^1y^3 + |E_{\{2,2\}}|x^2y^2 + |E_{\{2,3\}}|x^2y^3 + |E_{\{3,3\}}|x^3y^3 \\ &= 2xy^3 + (2a+1)x^2y^2 + (4a+8b-10)x^2y^3 + (12ab-8a-10b+7)x^3y^3. \end{aligned}$$

□



(a) (b)

Figure 5: Plotting M-polynomial of SiC_3-$II[4,3]$: range of (a) $-0.10 \leq x, y \leq 0.10$ and (b) $1 \leq x, y \leq 5$.

Figure 5 provides a visualization of the M-polynomial for SiC_3-$II[4,3]$ in range $-0.10 \leq x, y \leq 0.10$ and $1 \leq x, y \leq 5$.

Theorem 5. *Let SiC_3-$II[a,b]$ be a silicon-carbide network. Then, the topological indices are given as*

(i) $M_1(SiC_3\text{-}II[a,b]) = 72ab - 28a - 20b + 4$,

(ii) $M_2(SiC_3\text{-}II[a,b]) = 108ab - 48a - 42b + 13$,

(iii) ${}^{m}M_2(SiC_3\text{-}II[a,b]) = \frac{4}{3}ab + \frac{5}{18}a + \frac{2}{9}b + \frac{1}{36}$,

(iv) $R_\alpha(SiC_3\text{-}II[a,b]) = 2^\alpha 3^\alpha + 2^{2\alpha}(2a+1) + 2^\alpha 3^\alpha(4a+8b-10) + 3^{2\alpha}(12ab - 8a - 10b + 7)$,

(v) $RR_\alpha(SiC_3\text{-}II[a,b]) = \frac{2^\alpha}{3^\alpha} + \frac{1}{2^{2\alpha}}(2a+1) + \frac{1}{2^\alpha 3^\alpha}(4a+8b-10) + \frac{1}{3^{2\alpha}}(12ab - 8a - 10b + 7)$,

(vi) $SDD(SiC_3\text{-}II[a,b]) = 24ab - \frac{10}{3}a - \frac{8}{3}b + 1$,

(vii) $H(SiC_3\text{-}II[a,b]) = 4ab - \frac{2}{5}a - \frac{2}{15}b - \frac{1}{6}$,

(viii) $ISI(SiC_3\text{-}II[a,b]) = 18ab - \frac{26}{5}a - \frac{27}{5}b + 1$,

(ix) $AZI(SiC_3\text{-}II[a,b]) = \frac{2187}{16}ab - \frac{345}{8}a - \frac{3194}{64}b + \frac{2223}{64}$.

Proof. Based on the Theorem 4, we have the M-polynomial for SiC_3-$II[a,b]$ as

$$\begin{aligned} M(SiC_3\text{-}II[a,b];x,y) =& 2xy^3+(2a+1)x^2y^2+(4a+8b-10)x^2y^3 \\ &+(12ab-8a-10b+7)x^3y^3. \end{aligned}$$

We denote $q(x,y)=M(SiC_3\text{-}II[a,b];x,y)$ for notational convenience. Let us now compute the following terms which will be used for determining the topological indices.

- $D_x(q(x,y))=2xy^3+2(2a+1)x^2y^2+2(4a+8b-10)x^2y^3+3(12ab-8a-10b+7)x^3y^3$,
- $D_y(q(x,y))=6xy^3+2(2a+1)x^2y^2+3(4a+8b-10)x^2y^3+3(12ab-8a-10b+7)x^3y^3$,
- $D_xD_y(q(x,y))=6xy^3+4(2a+1)x^2y^2+6(4a+8b-10)x^2y^3+9(12ab-8a-10b+7)x^3y^3$,
- $S_x(q(x,y))=2xy^3+\frac{1}{2}(2a+1)x^2y^2+\frac{1}{2}(4a+8b-10)x^2y^3+\frac{1}{3}(12ab-8a-10b+7)x^3y^3$,
- $S_y(q(x,y))=\frac{2}{3}xy^3+\frac{1}{2}(2a+1)x^2y^2+\frac{1}{3}(4a+8b-10)x^2y^3+\frac{1}{3}(12ab-8a-10b+7)x^3y^3$,
- $S_xS_y(q(x,y))=\frac{2}{3}xy^3+\frac{1}{4}(2a+1)x^2y^2+\frac{1}{6}(4a+8b-10)x^2y^3+\frac{1}{9}(12ab-8a-10b+7)x^3y^3$,
- $D_x^{\alpha}D_y^{\alpha}(q(x,y))=2^{\alpha}3^{\alpha}xy^3+2^{2\alpha}(2a+1)x^2y^2+2^{\alpha}3^{\alpha}(4a+8b-10)x^2y^3+3^{2\alpha}(12ab-8a-10b+7)x^3y^3$,
- $D_xS_y(q(x,y))=\frac{2}{3}xy^3+(2a+1)x^2y^2+\frac{2}{3}(4a+8b-10)x^2y^3+(12ab-8a-10b+7)x^3y^3$,
- $D_yS_x(q(x,y))=6xy^3+(2a+1)x^2y^2+\frac{3}{2}(4a+8b-10)x^2y^3+(12ab-8a-10b+7)x^3y^3$,
- $S_x^{\alpha}S_y^{\alpha}(q(x,y))=\frac{2^{\alpha}}{3^{\alpha}}xy^3+\frac{1}{2^{2\alpha}}(2a+1)x^2y^2+\frac{1}{2^{\alpha}3^{\alpha}}(4a+8b-10))x^2y^3+\frac{1}{3^{2\alpha}}(12ab-8a-10b+7)x^3y^3$,
- $S_xJ(q(x,y))=\frac{1}{4}(3+2a)x^4+\frac{1}{5}(4a+8b-10)x^5+\frac{1}{6}(12ab-8a-10b+7)x^6$,
- $S_xJD_xD_y(q(x,y))=\frac{1}{4}(10+8a)x^4+\frac{1}{5}(24a+48b-60)x^5+\frac{1}{6}(108ab-72a-90b+63)x^6$,

- $S_x^3 Q_{-2} J D_x^3 D_y^3(q(x,y)) = (3^3 + 2^3(2a+1))x^2 + 2^3(4a+8b-10)x^3 + \frac{3^6}{4^3}(12ab - 8a - 10b + 7)x^4$.

Hence, the nine topological indices for SiC_3-$II[a,b]$ derived from the established formulas are as follows

(i) $M_1(SiC_3\text{-}II[a,b]) = (D_x + D_y)(q(x,y))|_{x=y=1} = 72ab - 28a - 20b + 4$,

(ii) $M_2(SiC_3\text{-}II[a,b]) = (D_x D_y)(q(x,y))|_{x=y=1} = 108ab - 48a - 42b + 13$,

(iii) ${}^m M_2(SiC_3\text{-}II[a,b]) = (S_x S_y)(q(x,y))|_{x=y=1} = \frac{4}{3}ab + \frac{5}{18}a + \frac{2}{9}b + \frac{1}{36}$,

(iv) $R_\alpha(SiC_3\text{-}II[a,b]) = (D_x^\alpha D_y^\alpha)(q(x,y))|_{x=y=1} = 2^{2\alpha}3^\alpha + 2^{2\alpha}(2a+1) + 2^\alpha 3^\alpha(4a+8b-10) + 3^{2\alpha}(12ab - 8a - 10b + 7)$,

(v) $RR_\alpha(SiC_3\text{-}II[a,b]) = (S_x^\alpha S_y^\alpha)(q(x,y))|_{x=y=1} = \frac{2^\alpha}{3^\alpha} + \frac{1}{2^\alpha}(2a+1) + \frac{1}{2^\alpha 3^\alpha}(4a + 8b - 10) + \frac{1}{3^{2\alpha}}(12ab - 8a - 10b + 7)$,

(vi) $SDD(SiC_3\text{-}II[a,b]) = (D_x S_y + D_y S_x)(q(x,y))|_{x=y=1} = 24ab - \frac{10}{3}a - \frac{8}{3}b + 1$,

(vii) $H(SiC_3\text{-}II[a,b]) = 2S_x J(q(x,y))|_{x=1} = 4ab - \frac{2}{5}a - \frac{2}{15}b - \frac{1}{6}$,

(viii) $ISI(SiC_3\text{-}II[a,b]) = S_x J D_x D_y(q(x,y))|_{x=1} = 18ab - \frac{26}{5}a - \frac{27}{5}b + 1$,

(ix) $AZI(SiC_3\text{-}II[a,b]) = S_x^3 Q_{-2} J D_x^3 D_y^3(q(x,y))|_{x=1} = \frac{2187}{16}ab - \frac{345}{8}a - \frac{3194}{64}b + \frac{2223}{64}$.

□

2.2.2 Visualizing Topological Indices of SiC_3-$II[a,b]$

Table 4 represents the M-polynomial and the associated indices for different parameters a and b in the SiC_3-$II[a,b]$ structure. To analyze the behavior of the M-polynomial and associated indices, we examine parameter values of a and b ranging from $a = 2$ to $a = 4$ and $b = 1$ to $b = 3$. Figure 6 displays the visualization of topological indices for SiC_3-$II[a,b]$ over the ranges $2 \leq a \leq 100$ and $1 \leq b \leq 100$ using MATLAB R2022a. The results display the values of all topological indices exhibit increasing values with simultaneous increase of a and b.

Table 4: Computation of nine topological indices of SiC_3-$II[a,b]$ by deriving the M-polynomial for various values of a and b.

Sl.	$[a,b]$	$[2,1]$	$[2,2]$	$[2,3]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
	M-polynomial / Topological Index	$2xy^3 + 5x^2y^2 + 6x^2y^3 + 5x^3y^3$	$2xy^3 + 5x^2y^2 + 14x^2y^3 + 19x^3y^3$	$2xy^3 + 5x^2y^2 + 22x^2y^3 + 33x^3y^3$	$2xy^3 + 7x^2y^2 + 10x^2y^3 + 9x^3y^3$	$2xy^3 + 7x^2y^2 + 18x^2y^3 + 35x^3y^3$	$2xy^3 + 7x^2y^2 + 18x^2y^3 + 61x^3y^3$	$2xy^3 + 9x^2y^2 + 14x^2y^3 + 13x^3y^3$	$2xy^3 + 9x^2y^2 + 22x^2y^3 + 51x^3y^3$	$2xy^3 + 9x^2y^2 + 30x^2y^3 + 89x^3y^3$
1.	First Zagreb Index	72	196	320	116	312	508	160	428	696
2.	Second Zagreb Index	91	265	439	151	433	715	211	601	991
3.	Modified Second Zagreb Index	3.4722	6.3611	9.2500	5.0833	9.3056	13.5278	6.6944	12.2500	17.8056
4.	General Randić Index ($\alpha = -1/2$)	7.0244	14.9571	22.8897	10.9907	22.9234	34.8560	14.9571	30.8897	46.8224
5.	Inverse Randić Index ($\alpha = -1/2$)	40.9217	102.5176	164.1135	66.7196	164.3156	261.9115	92.5176	226.1135	359.7094
6.	Symmetric Division (Deg) Index	39.6667	85.0000	130.3333	60.3333	129.6667	199.0000	81.0000	174.3333	267.6667
7.	Harmonic Index	6.9000	14.7667	22.6333	10.5000	22.3667	34.2333	14.1000	29.9667	45.8333
8.	Inverse Sum (Indeg) Index	21.2000	51.8000	82.4000	34.0000	82.6000	131.2000	46.8000	113.4000	180.0000
9.	Augmented Zagreb Index	171.9531	395.4219	618.8906	265.5156	625.6719	985.8281	359.0781	855.9219	1352.8000

2.3 Silicon-Carbide Network SiC_3-$III[a,b]$

The molecular structure of silicon-carbide SiC_3-$III[a,b]$, for $a = 5$ and $b = 4$ is shown in Figure 7. The graph of SiC_3-$III[a,b]$ consists of $8ab$ vertices and $12ab - 3a - 2b$ edges.

2.3.1 Evaluating the M-polynomial for SiC_3-$III[a,b]$

Theorem 6. *Let SiC_3-$III[a,b]$ be a silicon-carbide network with $a > 1, b \geq 1$. Then, the M-polynomial of SiC_3-$III[a,b]$ is given by*

$$M(SiC_3\text{-}III[a,b];x,y) = 2xy^2 + xy^3 + (3a+2b-3)x^2y^2 + (6a+4b-8)x^2y^3 + (12ab-12a-8b+8)x^3y^3.$$

Proof. As above for the structure of silicon-carbide SiC_3-$III[a,b]$, we have

$$|V| = 8ab \quad \text{and} \quad |E| = 12ab - 3a - 2b.$$

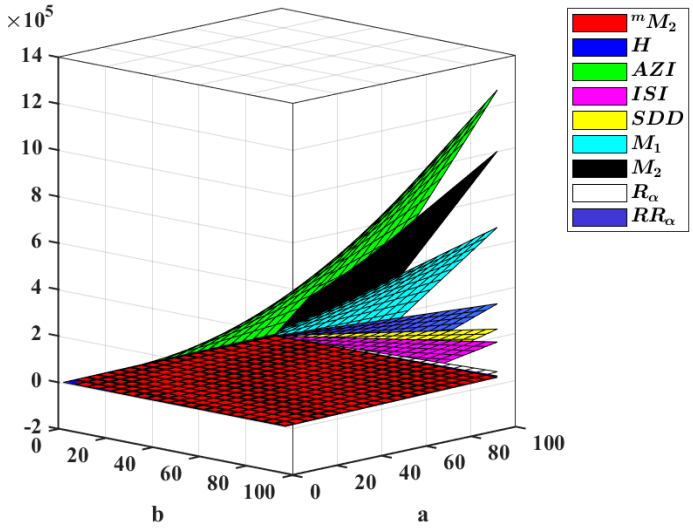


Figure 6: Plotting different parameters a and b ($2 \leq a \leq 100$ and $1 \leq b \leq 100$) of SiC_3-$II[a, b]$ for all nine indices.

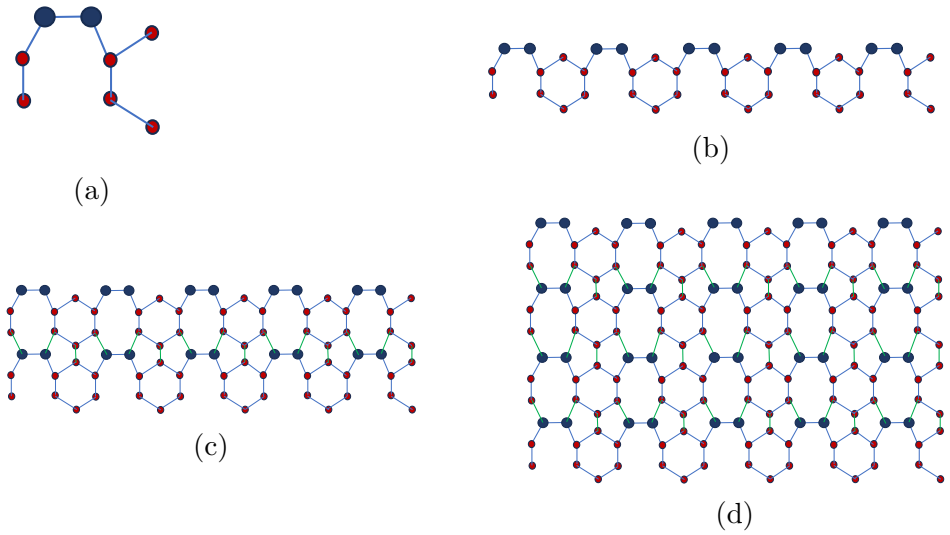


Figure 7: (a) The unit cell of SiC_3-$III[a, b]$, (b) The molecular structure of SiC_3-$III[5, 1]$, (c) SiC_3-$III[5, 2]$, and (d) SiC_3-$III[5, 4]$.

Now, the values for the five partitions determined by the degree of each edge's terminal vertices are calculated as

$$\begin{aligned}
E_1 = E_{\{1,2\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}III[a,b]) : d_{u_1} = 1, d_{u_2} = 2\},\\
E_2 = E_{\{1,3\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}III[a,b]) : d_{u_1} = 1, d_{u_2} = 3\},\\
E_3 = E_{\{2,2\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}III[a,b]) : d_{u_1} = 2, d_{u_2} = 2\},\\
E_4 = E_{\{2,3\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}III[a,b]) : d_{u_1} = 2, d_{u_2} = 3\},\\
\text{and}\quad E_5 = E_{\{3,3\}} &= \{e = u_1u_2 \in E(SiC_3\text{-}III[a,b]) : d_{u_1} = 3, d_{u_2} = 3\}.
\end{aligned}$$

Now, we have $|E_1| = 2$, $|E_2| = 1$, $|E_3| = 3a + 2b - 3$,$|E_4| = 6a + 4b - 8$ and $|E_5| = 12ab - 12a - 8b + 8$ for $a > 1, b \geq 1$. Therefore by definition, the M-polynomial of $SiC_3\text{-}III[a,b]$ is

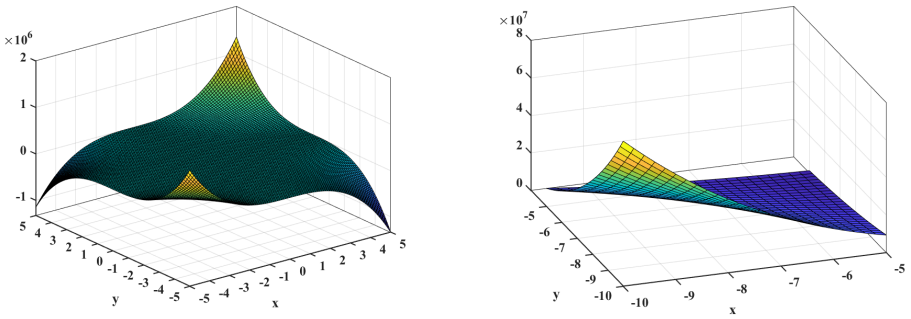
$$\begin{aligned}
&M(SiC_3\text{-}III[a,b]; x, y)\\
&= \sum_{i\leq j} m_{i,j}x^iy^j, \quad \text{where} \quad i,j \in \{1,2,3\}\\
&= \sum_{1\leq 2} m_{1,2}x^1y^2 + \sum_{1\leq 3} m_{1,3}x^1y^3 + \sum_{2\leq 2} m_{2,2}x^2y^2 + \sum_{2\leq 3} m_{2,3}x^2y^3 + \sum_{3\leq 3} m_{3,3}x^3y^3\\
&= \sum_{u_1u_2\in E_1(SiC_3\text{-}III[a,b])} m_{1,2}x^1y^2 + \sum_{u_1u_2\in E_2(SiC_3\text{-}III[a,b])} m_{1,3}xy^3 +\\
&\quad \sum_{u_1u_2\in E_3(SiC_3\text{-}III[a,b])} m_{2,2}x^2y^2 + \sum_{u_1u_2\in E_4(SiC_3\text{-}III[a,b])} m_{2,3}x^2y^3 +\\
&\quad \sum_{u_1u_2\in E_5(SiC_3\text{-}III[a,b])} m_{3,3}x^3y^3\\
&= |E_{\{1,2\}}|x^1y^2 + |E_{\{1,3\}}|x^1y^3 + |E_{\{2,2\}}|x^2y^2 + |E_{\{2,3\}}|x^2y^3 + |E_{\{3,3\}}|x^3y^3\\
&= 2xy^2 + xy^3 + (3a + 2b - 3)x^2y^2 + (6a + 4b - 8)x^2y^3\\
&+ (12ab - 12a - 8b + 8)x^3y^3.
\end{aligned}$$

□

Figure 8 provides a visualization of the M-polynomial for $SiC_3\text{-}III[5,4]$ in range $-5 \leq x, y \leq 5$ and $-10 \leq x, y \leq -5$.

Theorem 7. *Let $SiC_3\text{-}III[a,b]$ be a silicon-carbide network. Then, the topological indices are given as*

(i) $M_1(SiC_3\text{-}III[a,b]) = 72ab - 30a - 20b + 6$,



(a) (b)

Figure 8: Plotting M-polynomial of SiC_3-$III[5,4]$: range of (a) $-5 \leq x, y \leq 5$ and (b) $-10 \leq x, y \leq -5$.

(ii) $M_2(SiC_3\text{-}III[a,b]) = 108ab - 60a - 40b + 19$,

(iii) ${}^{m}M_2(SiC_3\text{-}III[a,b]) = \frac{4}{3}ab + \frac{5}{12}a + \frac{5}{18}b + \frac{5}{36}$,

(iv) $R_\alpha(SiC_3\text{-}III[a,b]) = 2^{2\alpha} + 3^\alpha + 2^{2\alpha}(3a + 2b - 3) + 2^\alpha 3^\alpha(6a + 4b - 8) + 3^{2\alpha}(12ab - 12a - 8b + 8)$,

(v) $RR_\alpha(SiC_3\text{-}III[a,b]) = 1 + \frac{1}{3^\alpha} + \frac{1}{2^{2\alpha}}(3a + 2b - 3) + \frac{1}{2^\alpha 3^\alpha}(6a + 4b - 8) + \frac{1}{3^{2\alpha}}(12ab - 12a - 8b + 8)$,

(vi) $SDD(SiC_3\text{-}III[a,b]) = 24ab - 5a - \frac{10}{3}b + \frac{55}{3}$,

(vii) $H(SiC_3\text{-}III[a,b]) = 4ab - \frac{1}{10}a - \frac{1}{15}b - \frac{1}{5}$,

(viii) $ISI(SiC_3\text{-}III[a,b]) = 18ab - \frac{39}{5}a - \frac{26}{5}b + \frac{56}{15}$,

(ix) $AZI(SiC_3\text{-}III[a,b]) = \frac{2187}{16}ab - \frac{1035}{16}a - \frac{345}{8}b + \frac{564}{8}$.

Proof. As computed in Theorem 6, we have the M-polynomial for SiC_3-$III[a,b]$ as

$$M(SiC_3\text{-}III[a,b];x,y) = 2xy^2 + xy^3 + (3a + 2b - 3)x^2y^2 + (6a + 4b - 8)x^2y^3 + (12ab - 12a - 8b + 8)x^3y^3.$$

We denote $q(x,y) = M(SiC_3\text{-}III[a,b];x,y)$ for notational convenience. The following operators are applied over $q(x,y)$.

- $D_x(q(x,y)) = 2xy^2 + xy^3 + 2(3a+2b-3)x^2y^2 + 2(6a+4b-8)x^2y^3 + 3(12ab-12a-8b+8)x^3y^3$,
- $D_y(q(x,y)) = 4xy^2 + 3xy^3 + 2(3a+2b-3)x^2y^2 + 3(6a+4b-8))x^2y^3 + 3(12ab-12a-8b+8)x^3y^3$,
- $D_xD_y(q(x,y)) = 4xy^2+3xy^3+4(3a+2b-3)x^2y^2+6(6a+4b-8))x^2y^3+9(12ab-12a-8b+8)x^3y^3$,
- $S_x(q(x,y)) = 2xy^2 + xy^3 + \frac{1}{2}(3a+2b-3)x^2y^2 + \frac{1}{2}(6a+4b-8)x^2y^3 + \frac{1}{3}(12ab-12a-8b+8)x^3y^3$,
- $S_y(q(x,y)) = xy^2 + \frac{1}{3}xy^3 + \frac{1}{2}(3a+2b-3)x^2y^2 + \frac{1}{3}(6a+4b-8))x^2y^3 + \frac{1}{3}(12ab-12a-8b+8)x^3y^3$,
- $S_xS_y(q(x,y)) = xy^2 + \frac{1}{3}xy^3 + \frac{1}{4}(3a+2b-3)x^2y^2 + \frac{1}{6}(6a+4b-8)x^2y^3 + \frac{1}{9}(12ab-12a-8b+8)x^3y^3$,
- $D_x^{\alpha}D_y^{\alpha}(q(x,y)) = 2^{2\alpha}xy^2 + 3^{\alpha}xy^3 + 2^{2\alpha}(3a+2b-3)x^2y^2 + 2^{\alpha}3^{\alpha}(6a+4b-8)x^2y^3 + 3^{2\alpha}(12ab-12a-8b+8)x^3y^3$,
- $D_xS_y(q(x,y)) = xy^2 + \frac{1}{3}xy^3 + (3a+2b-3)x^2y^2 + \frac{2}{3}(6a+4b-8))x^2y^3 + (12ab-12a-8b+8)x^3y^3$,
- $D_yS_x(q(x,y)) = 4xy^2 + 3xy^3 + (3a+2b-3)x^2y^2 + \frac{3}{2}(6a+4b-8)x^2y^3 + (12ab-12a-8b+8)x^3y^3$,
- $S_x^{\alpha}S_y^{\alpha}(q(x,y)) = xy^2 + \frac{1}{3^{\alpha}}xy^3 + \frac{1}{2^{2\alpha}}(3a+2b-3)x^2y^2 + \frac{1}{2^{\alpha}3^{\alpha}}(6a+4b-8))x^2y^3 + \frac{1}{3^{2\alpha}}(12ab-12a-8b+8)x^3y^3$,
- $S_xJ(q(x,y)) = \frac{2}{3}x^3 + \frac{1}{4}(3a+2b-2)x^4 + \frac{1}{5}(6a+4b-8))x^5 + \frac{1}{6}(12ab-12a-8b+8)x^6$,
- $S_xJD_xD_y(q(x,y)) = \frac{4}{3}x^3 + (3a+2b)x^4 + \frac{6}{5}(6a+4b-8))x^5 + \frac{9}{6}(12ab-12a-8b+8)x^6$,
- $S_x^3Q_{-2}JD_x^3D_y^3(q(x,y)) = 2^6x + \frac{3^3}{2^3}x^2 + 2^3(3a+2b-3)x^2 + 2^3(6a+4b-8)x^3 + \frac{3^6}{4^3}(12ab-12a-8b+8)x^6$.

Hence, the nine topological indices for SiC_3-$III[a,b]$ derived from the established formulas are given below

(i) $M_1(SiC_3\text{-}III[a,b]) = (D_x+D_y)(q(x,y))|_{x=y=1} = 72ab-30a-20b+6$,

(ii) $M_2(SiC_3\text{-}III[a,b]) = (D_xD_y)(q(x,y))|_{x=y=1} = 108ab - 60a - 40b + 19$,

(iii) ${}^mM_2(SiC_3\text{-}III[a,b]) = (S_xS_y)(q(x,y))|_{x=y=1} = \frac{4}{3}ab + \frac{5}{12}a + \frac{5}{18}b + \frac{5}{36}$,

(iv) $R_\alpha(SiC_3\text{-}III[a,b]) = (D_x^\alpha D_y^\alpha)(q(x,y))|_{x=y=1} = 2^{2\alpha} + 3^\alpha + 2^{2\alpha}(3a+2b-3) + 2^\alpha 3^\alpha(6a+4b-8)) + 3^{2\alpha}(12ab - 12a - 8b + 8)$,

(v) $RR_\alpha(SiC_3\text{-}III[a,b]) = (S_x^\alpha S_y^\alpha)(q(x,y))|_{x=y=1} = 1 + \frac{1}{3^\alpha} + \frac{1}{2^{2\alpha}}(3a+2b-3) + \frac{1}{2^\alpha 3^\alpha}(6a+4b-8)) + \frac{1}{3^{2\alpha}}(12ab - 12a - 8b + 8)$,

(vi) $SDD(SiC_3\text{-}III[a,b]) = (D_xS_y + D_yS_x)(q(x,y))|_{x=y=1} = 24ab - 5a - \frac{10}{3}b + \frac{55}{3}$,

(vii) $H(SiC_3\text{-}III[a,b]) = 2S_xJ(q(x,y))|_{x=1} = 4ab - \frac{1}{10}a - \frac{1}{15}b - \frac{1}{5}$,

(viii) $ISI(SiC_3\text{-}III[a,b]) = S_xJD_xD_y(q(x,y))|_{x=1} = 18ab - \frac{39}{5}a - \frac{26}{5}b + \frac{56}{15}$,

(ix) $AZI(SiC_3\text{-}III[a,b]) = S_x^3Q_{-2}JD_x^3D_y^3(q(x,y))|_{x=1} = \frac{2187}{16}ab - \frac{1035}{16}a - \frac{345}{8}b + \frac{564}{8}$.

□

2.3.2 Visualizing Topological Indices of $SiC_3\text{-}III[a,b]$

For the different parameters a and b, the M-polynomial and the associated indices are represented by Table 5. To analyze the behavior of the M-polynomial and corresponding indices, we examine the parameter values ranging from $a = 2$ to $a = 4$ and $b = 1$ to $b = 3$. Figure 9 displays the visualization of nine topological indices for $SiC_3\text{-}III[5,4]$ over the ranges $2 \le a \le 100$ and $1 \le b \le 100$ using MATLAB R2022a software. The results demonstrate that all topological indices exhibit increasing values with simultaneous increase of parameters a and b.

3 Comparative Analysis among the Topological Indices

In this section, we perform a comparative analysis by analyzing the behavior of nine degree-based topological indices for the silicon-carbide networks $SiC_3\text{-}I[a,b]$, $SiC_3\text{-}II[a,b]$ and $SiC_3\text{-}III[a,b]$ across different values of a and b. For each structures, we represent the graphs of the topological indices shown in Figures 3, 6 and 9 and the corresponding computational values,

Table 5: Computation of nine topological indices of SiC_3-$III[a,b]$ by deriving the M-polynomial for various values of a and b.

Sl.	$[a,b]$	$[2,1]$	$[2,2]$	$[2,3]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
	M-polynomial / Topological Index	$2xy^2 + 5x^2y^2 + xy^3 + 8x^2y^3$	$2xy^2 + 7x^2y^2 + xy^3 + 12x^2y^3 + 16x^3y^3$	$2xy^2 + 9x^2y^2 + xy^3 + 16x^2y^3 + 32x^3y^3$	$2xy^2 + 8x^2y^2 + xy^3 + 14x^2y^3$	$2xy^2 + 10x^2y^2 + xy^3 + 18x^2y^3 + 28x^3y^3$	$2xy^2 + 12x^2y^2 + xy^3 + 22x^2y^3 + 56x^3y^3$	$2xy^2 + 11x^2y^2 + xy^3 + 20x^2y^3$	$2xy^2 + 13x^2y^2 + xy^3 + 24x^2y^3 + 40x^3y^3$	$2xy^2 + 15x^2y^2 + xy^3 + 28x^2y^3 + 80x^3y^3$
1.	First Zagreb Index	70	194	318	112	308	504	154	422	690
2.	Second Zagreb Index	75	251	427	123	407	691	171	563	955
3.	Modified Second Zagreb Index	3.9167	6.8611	9.8056	5.6667	9.9444	14.2222	7.4167	13.0278	18.6389
4.	General Randić Index ($\alpha = -1/2$)	6.5993	14.5656	22.5320	10.5488	22.5151	34.4815	14.4983	30.4646	46.4310
5.	Inverse Randić Index ($\alpha = -1/2$)	30.5959	92.3939	154.1918	51.2929	149.0908	246.8888	71.9898	205.7878	339.5857
6.	Symmetric Division (Deg) Index	53.0000	97.6667	142.3333	72.0000	140.6667	209.3333	91.0000	183.6667	276.3333
7.	Harmonic Index	7.5333	15.4667	23.4000	11.4333	23.3667	35.3000	15.3333	31.2667	47.2000
8.	Inverse Sum (Indeg) Index	18.9333	49.7333	80.5333	29.1333	77.9333	126.7333	39.3333	106.1333	172.9333
9.	Augmented Zagreb Index	171.3750	401.6250	631.8750	243.3750	610.3125	977.2500	315.3750	819.0000	1322.6000

where parameter values ranging from $a = 2$ to $a = 4$ and $b = 1$ to $b = 3$, are provided in Tables 3, 4 and 5.

Based on these computations, we observe the following relationships for each network.

(i) For SiC_3-$I[a,b]$ network, when the parameter ranges from $a = 2$ to $a = 4$ and $b = 2$ to $b = 3$.

$$^mM_2 < R_{-\frac{1}{2}} < H < ISI < SDD < RR_{-\frac{1}{2}} < M_1 < M_2 < AZI.$$

(ii) For SiC_3-$II[a,b]$ network, when the parameter ranges from $a = 2$ to $a = 4$ and $b = 1$ to $b = 3$.

$$^mM_2 < H < R_{-\frac{1}{2}} < ISI < SDD < RR_{-\frac{1}{2}} < M_1 < M_2 < AZI.$$

(iii) For SiC_3-$III[a,b]$ network, when the parameter ranges from $a = 2$ to $a = 3$ and $b = 1$ to $b = 3$.

$$^mM_2 < R_{-\frac{1}{2}} < H < ISI < RR_{-\frac{1}{2}} < SDD < M_1 < M_2 < AZI.$$

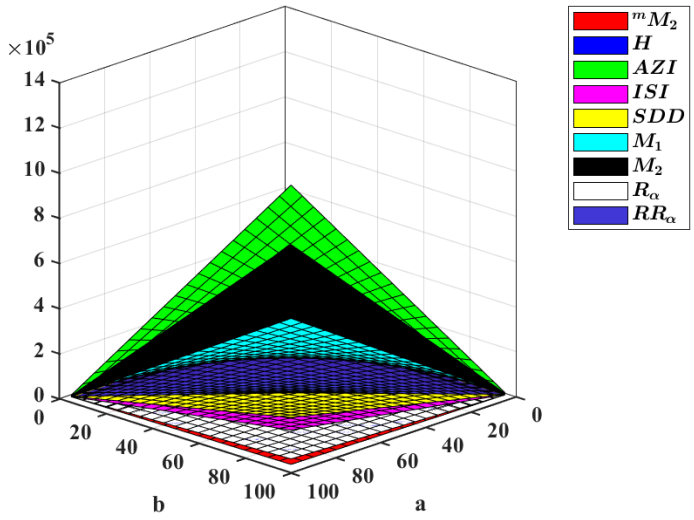


Figure 9: Plotting different parameters a and b ($2 \leq a \leq 100$ and $1 \leq b \leq 100$) of SiC_3-$III[5, 4]$ for all nine indices.

When the parameter ranges from $a = 3$ to $a = 4$ and $b = 1$ to $b = 3$, we have

$$^{m}M_2 < R_{-\frac{1}{2}} < H < ISI < SDD < RR_{-\frac{1}{2}} < M_1 < M_2 < AZI.$$

Further for the comparative analysis, the computational values for all topological indices across these three networks, particularly for $a = b$ ($2 \leq a, b \leq 10$), are enumerated in Tables 6, 7 and 8. Under these conditions, we observe the following ordered relationships.

(i) For the structures SiC_3-$I[a, b]$ and SiC_3-$III[a, b]$, we get

$$^{m}M_2 < R_{-\frac{1}{2}} < H < ISI < SDD < RR_{-\frac{1}{2}} < M_1 < M_2 < AZI.$$

(ii) For the structure SiC_3-$II[a, b]$, we get

$$^{m}M_2 < H < R_{-\frac{1}{2}} < ISI < SDD < RR_{-\frac{1}{2}} < M_1 < M_2 < AZI.$$

These results show that, the modified second Zagreb index ($^{m}M_2$) exhibits the minimum value, whereas the augmented Zagreb index (AZI) exhibits the

Table 6: Computing the topological indices of SiC_3-$I[a,b]$ when $a = b$ ($2 \leq a, b \leq 10$).

Sl.	Topological Index / $[a,b]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$	$[8,8]$	$[9,9]$	$[10,10]$
1.	**First Zagreb Index**	194	504	958	1556	2298	3184	4214	5388	6706
2.	**Second Zagreb Index**	249	688	1343	2214	3301	4604	6123	7858	9809
3.	**Modified Second Zagreb Index**	6.8056	14.1389	24.1389	36.8056	52.1389	70.1389	90.8056	114.1389	140.1389
4.	**General Randić Index** ($\alpha = -1/2$)	14.5320	34.4310	62.3299	98.2289	142.1279	194.0269	253.9258	321.8248	397.7238
5.	**Inverse Randić Index** ($\alpha = -1/2$)	93.9239	248.3178	474.7116	773.1055	1143.5000	1585.9000	2100.3000	2686.7000	3345.1000
6.	**Symmetric Division (Deg) Index**	81	193	353	561	817	1121	1473	1873	2321
7.	**Harmonic Index**	15.4000	35.2000	63.0000	98.8000	142.6000	194.4000	254.2000	322	397.8000
8.	**Inverse Sum (Indeg) Index**	47.2833	124.1833	237.0833	385.9833	570.8833	791.7833	1048.7000	1341.6000	1670.5000
9.	**Augmented Zagreb Index**	394.8438	967.0781	1812.7000	2931.7000	4324.0000	5989.8000	7928.9000	10141.000	12627.000

maximum value across all three networks. Additionally, comparing Tables 3, 4 and 5 with Tables 6, 7 and 8 reveals that, these ordered relationships remain same as we increase the parameter values (in the domain $2 \leq a, b \leq 10$) excluding SDD and $RR_{-\frac{1}{2}}$ which changes ordering at parameter values $a = 2$ to $a = 3$ and $b = 1$ to $b = 3$ for SiC_3-$III[a,b]$ network. For each of the silicon-carbide structures shown in Figure 10, which are drawn using MATLAB R2022a software, we analyze the following observations given below.

(i) For the first Zagreb index M_1:

$$TI(SiC_3\text{-}I) = TI(SiC_3\text{-}III) < TI(SiC_3\text{-}II).$$

Table 7: Computing the topological indices of SiC_3-$II[a,b]$ when $a = b$ $(2 \leq a, b \leq 10)$.

Sl.	Topological Index / $[a,b]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$	$[8,8]$	$[9,9]$	$[10,10]$
1.	**First Zagreb Index**	196	508	964	1564	2308	3196	4228	5404	6724
2.	**Second Zagreb Index**	265	715	1381	2263	3361	4675	6205	7951	9913
3.	**Modified Second Zagreb Index**	6.3611	13.5278	23.3611	35.8611	51.0278	68.8611	89.3611	112.5278	138.3611
4.	**General Randić Index** ($\alpha = -1/2$)	14.9571	34.8560	62.7550	98.6540	142.5530	194.4520	254.3509	322.2499	398.1489
5.	**Inverse Randić Index** ($\alpha = -1/2$)	102.5176	261.9115	493.3054	796.6992	1172.1000	1619.5000	2138.9000	2730.3000	3393.7000
6.	**Symmetric Division (Deg) Index**	85	199	361	571	829	1135	1489	1891	2341
7.	**Harmonic Index**	14.7667	34.2333	61.7000	97.1667	140.6333	192.1000	251.5667	319.0333	394.5000
8.	**Inverse Sum (Indeg) Index**	51.8000	131.2000	246.6000	398	585.4000	808.8000	1068.2000	1363.6000	1695
9.	**Augmented Zagreb Index**	395.4219	985.8281	1849.6000	2986.8000	4397.3000	6081.2000	8038.5000	10269.000	12773.000

(ii) For $M_2, R_{-\frac{1}{2}}, SDD, ISI,$ and AZI indices:

$$TI(SiC_3\text{-}I) < TI(SiC_3\text{-}III) < TI(SiC_3\text{-}II).$$

(iii) For $RR_{-\frac{1}{2}}$ index:

$$TI(SiC_3\text{-}III) < TI(SiC_3\text{-}I) < TI(SiC_3\text{-}II).$$

(iv) For ${}^{m}M_2$ and H indices:

$$TI(SiC_3\text{-}II) < TI(SiC_3\text{-}I) < TI(SiC_3\text{-}III).$$

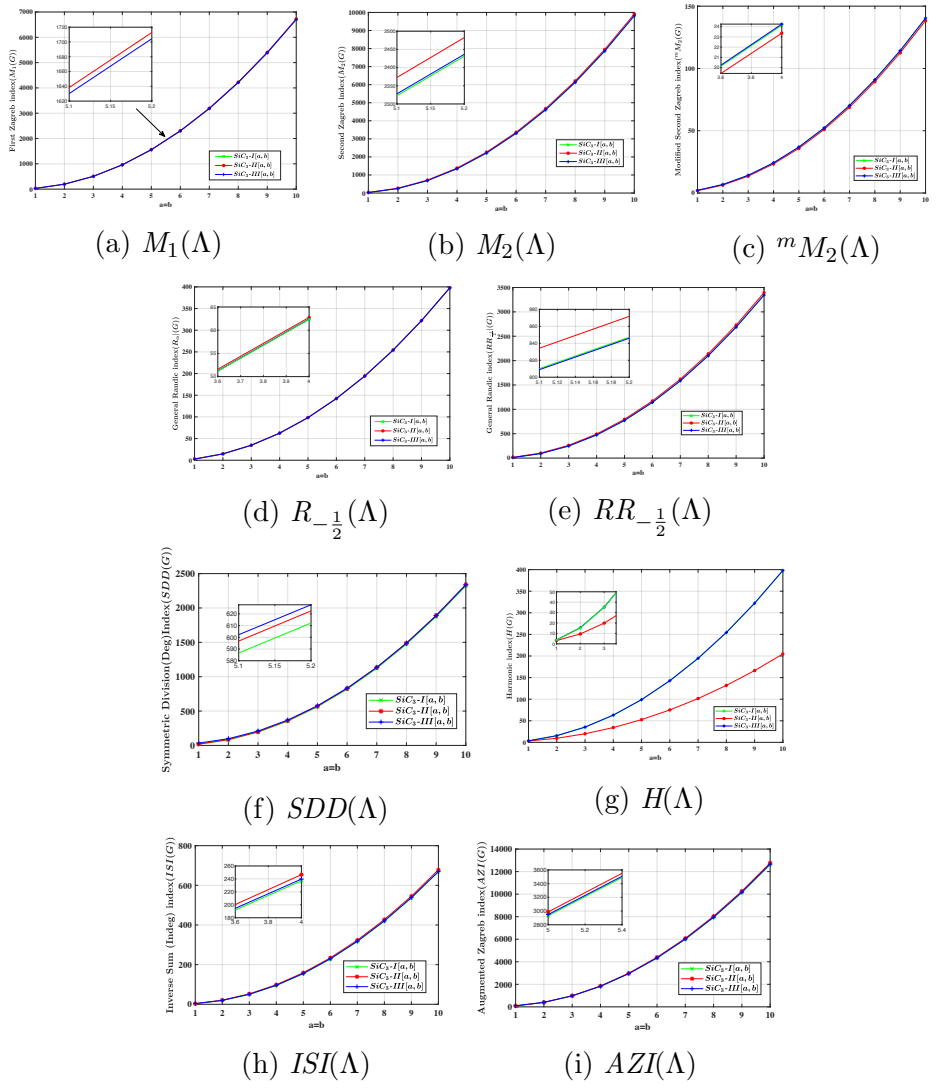
That is, the SiC_3-$I[a,b]$ and SiC_3-$III[a,b]$ networks yield same values for the M_1 index, whereas SiC_3-$II[a,b]$ network shows higher values than those

Table 8: Computing the topological indices of SiC_3-$III[a,b]$ when $a = b$ $(2 \leq a, b \leq 10)$.

Sl.	Topological Index / $[a,b]$	$[2,2]$	$[3,3]$	$[4,4]$	$[5,5]$	$[6,6]$	$[7,7]$	$[8,8]$	$[9,9]$	$[10,10]$
1.	**First Zagreb Index**	194	504	958	1556	2298	3184	4214	5388	6706
2.	**Second Zagreb Index**	251	691	1347	2219	3307	4611	6131	7867	9819
3.	**Modified Second Zagreb Index**	6.8611	14.2222	24.2500	36.9444	52.3056	70.3333	91.0278	114.3889	140.4167
4.	**General Randić Index** ($\alpha = -1/2$)	14.5656	34.4815	62.3973	98.3131	142.2289	194.1447	254.0605	321.9764	397.8922
5.	**Inverse Randić Index** ($\alpha = -1/2$)	92.3939	246.8888	473.3837	771.8786	1142.4000	1584.9000	2099.4000	2685.9000	3344.4000
6.	**Symmetric Division (Deg) Index**	97.6667	209.3333	369.0000	576.6667	832.3333	1136.0000	1487.7000	1887.3000	2335.0000
7.	**Harmonic Index**	15.4667	35.3000	63.1333	98.9667	142.8000	194.6333	254.4667	322.3000	398.1333
8.	**Inverse Sum (Indeg) Index**	49.7333	126.7333	239.7333	388.7333	573.7333	794.7333	1051.7000	1344.7000	1673.7000
9.	**Augmented Zagreb Index**	401.6250	977.2500	1826.3000	2948.6000	4344.4000	6013.5000	7956.0000	10172.000	12661.000

two. We observe that this order is not preserved for the remaining indices due to their different mathematical formulations. Furthermore, the M_2, $R_{-\frac{1}{2}}$, *SDD*, *ISI*, and *AZI* indices yield the highest values for SiC_3-$II[a,b]$ network and the lowest for the SiC_3-$I[a,b]$ network, with SiC_3-$III[a,b]$ lies between the two. Similarly, the $RR_{-\frac{1}{2}}$ index shows the highest for SiC_3-$II[a,b]$ and the lowest for SiC_3-$III[a,b]$, with SiC_3-$I[a,b]$ lies between the two. Additionally, the ${}^mM_2$ and H indices yield the highest for SiC_3-$III[a,b]$ and shows the lowest for SiC_3-$II[a,b]$, with SiC_3-$I[a,b]$ again lying between the two.

Furthermore, we compare our findings (obtained in Tables 3, 4 and 5) for SiC_3 with the existing literature [8] for Si_2C_3. In the article [8] (in Tables 4, 5 and 6), the authors tabulated the computational values of degree-based topological indices (namely, M_1, M_2, ${}^mM_2$, $R_{1/2}$, $RR_{1/2}$, *SDD*, H, *ISI*,



(a) $M_1(\Lambda)$ (b) $M_2(\Lambda)$ (c) ${}^{m}M_2(\Lambda)$

(d) $R_{-\frac{1}{2}}(\Lambda)$ (e) $RR_{-\frac{1}{2}}(\Lambda)$

(f) $SDD(\Lambda)$ (g) $H(\Lambda)$

(h) $ISI(\Lambda)$ (i) $AZI(\Lambda)$

Figure 10: Comparison between all considered indices of each of the networks SiC_3-$I[a,b]$, SiC_3-$II[a,b]$ and SiC_3-$III[a,b]$ when $a = b$.

and AZI) for $Si_2C_3[p,q]$ type networks. We observe the following ordered relationship for Si_2C_3-$I[p,q]$, Si_2C_3-$II[p,q]$ and Si_2C_3-$III[p,q]$ networks as follows.

$$^{m}M_2 < H < RR_{\frac{1}{2}} < ISI < SDD < R_{\frac{1}{2}} < M_1 < M_2 < AZI.$$

On comparing, we noted that this relationship for $Si_2C_3[p,q]$ networks is differ from our obtained relationships for $SiC_3[a,b]$ networks, and do not follow the same structural pattern. These observations reveal that the topological indices exhibit a specific ordering due to different structural patterns of the $SiC_3[a,b]$ networks. This ordering is not uniformly preserved across all computed topological indices due to their different vertex-and edge-based mathematical formulations.

Remark 8. *Regarding the relationship between the $Si_2C_3[p,q]$ and $SiC_3[a,b]$ networks, it is evident from the above arguments that they exhibit different structural patterns.*

4 Conclusion

In this study, the molecular graphs of silicon-carbide (SiC_3) type networks are analyzed. Rather than computing the degree-based topological indices individually, we derived closed-form expressions of the M-polynomial, allowing for the direct calculation of associated topological indices for each of the SiC_3-$I[a,b]$, SiC_3-$II[a,b]$ and SiC_3-$III[a,b]$ networks across different values of parameters a and b. Furthermore, we visually represented the M-polynomial and the associated indices for the different parameters across all three structures. Using the computational and graphical results, we conducted a comparative analysis among the considered topological indices, particularly at the parameters $a = b$ $(2 \leq a, b \leq 10)$ for these networks. The obtained results will provide a mathematical foundation for future researchers to investigate the chemical significance of these networks.

Acknowledgments

We sincerely thank the anonymous referees for the thorough reviews of this article of their valuable suggestions and comments which have helped us to improve the quality of the article. The second author also acknowledges financial support from Banaras Hindu University (BHU), Varanasi in the form of BHU-fellowship.

Author Contributions

All authors have contributed equally to the work done in the paper.

Data Availability Statement

The supporting data for these findings are presented in the article.

References

[1] Dragan Amić, Drago Bešlo, Bono Lucić, Sonja Nikolić, and Nenad Trinajstić. The Vertex-Connectivity Index Revisited. *Journal of Chemical Information and Computer Sciences*, 38(5):819–822, 1998. doi:10.1021/ci980039b.

[2] Micheal Arockiaraj, Francis Joseph H. Campena, A. Berin Greeni, Muhammad Usman Ghani, S. Gajavalli, Fairouz Tchier, and Ahmad Zubair Jan. QSPR analysis of distance-based structural indices for drug compounds in tuberculosis treatment. *Heliyon*, 10(2):e2405844024000124, 2024. doi:10.1016/j.heliyon.2024.e23981.

[3] Alexandru T. Balaban. Applications of graph theory in chemistry. *Journal of Chemical Information and Computer Sciences*, 25(3):334–343, 1985. doi:10.1021/ci00047a033.

[4] Deepa Balasubramaniyan, Natarajan Chidambaram, Vignesh Ravi, and Muhammad Kamran Siddiqui. QSPR analysis of anti-asthmatic drugs using some new distance-based topological indices: A comparative study. *International Journal of Quantum Chemistry*, 124(9):e27372, 2024. doi:10.1002/qua.27372.

[5] Jayjit Barman and Shibsankar Das. QSPR Analysis of Elliptic-type Entropy Measures and their Correlation with Elliptic-type Indices of Silicon Carbide Networks. *Silicon*, 18(6):2365–2390, 2026. doi:10.1007/s12633-026-03647-x.

[6] Béla Bollobás and Paul Erdös. Graphs of extremal weights. *Ars Combinatoria*, 50:225–233, 1998. URL: https://combinatorialpress.com/article/ars/Volume%20050/volume-50-paper-18.pdf.

[7] Gilles Caporossi, Ivan Gutman, Pierre Hansen, and Ljiljana Pavlović. Graphs with maximum connectivity index. *Computational Biology and Chemistry*, 27(1):85–90, 2003. doi:10.1016/S0097-8485(02)00016-5.

[8] Shibsankar Das and Virendra Kumar. On M-polynomial of the Two-dimensional Silicon-Carbons. *Palestine Journal of Mathematics*, 11(Special Issue II):136–157, 2022. URL: https://pjm.ppu.edu/paper/1035-m-polynomial-two-dimensional-silicon-carbons.

[9] Shibsankar Das and Virendra Kumar. Neighborhood degree sum-based molecular indices and their comparative analysis of some silicon carbide networks. *Physica Scripta*, 99(5):055941, 2024. doi:10.1088/1402-4896/ad3682.

[10] Shibsankar Das, Virendra Kumar, and Jayjit Barman. Geometric-Quadratic and Quadratic-Geometric Indices-based Entropy Measures of Silicon Carbide Networks. *Silicon*, 17(1):75–91, 2025. doi:10.1007/s12633-024-03173-8.

[11] Shibsankar Das and Shikha Rai. M-polynomial and related degree-based topological indices of the third type of chain Hex-derived network. *Malaya Journal of Matematik*, 8(4):1842–1850, 2020. doi:10.26637/MJM0804/0085.

[12] Shibsankar Das and Shikha Rai. M-polynomial and related degree-based topological indices of the third type of Hex-derived network. *Nanosystems: Physics, Chemistry, Mathematics*, 11(3):267–274, 2020. doi:10.17586/2220-8054-2020-11-3-267-274.

[13] Emeric Deutsch and Sandi Klavžar. M-polynomial and Degree-Based Topological Indices. *Iranian Journal of Mathematical Chemistry*, 6(2):93–102, 2015. doi:10.22052/ijmc.2015.10106.

[14] Edward J. Farrell. An introduction to matching polynomials. *Journal of Combinatorial Theory, Series B*, 27(1):75–86, 1979. doi:10.1016/0095-8956(79)90070-4.

[15] Boris Furtula, Ante Graovac, and Damir Vukičević. Augmented Zagreb index. *Journal of Mathematical Chemistry*, 48(2):370–380, 2010. doi:10.1007/s10910-010-9677-3.

[16] Ante Graovac, Ivan Gutman, Nenad Trinajstić, and Tomislav Živković. Graph theory and molecular orbitals: Application of Sachs theorem. *Theoretica Chimica Acta*, 26:67–78, 1972. doi:10.1007/BF00527654.

[17] Ivan Gutman. Some relations between distance-based polynomials of trees. *Bulletin (Ácadémie Serbe des Sciences et des Arts. Classe des Sciences Mathématiques et Naturelles. Sciences Mathématiques)*, pages 1–7, 2005. URL: http://www.jstor.org/stable/44095631.

[18] Ivan Gutman. Degree-based topological indices. *Croatica Chemica Acta*, 86(4):351–361, 2013. doi:10.5562/cca2294.

[19] Ivan Gutman and Nenad Trinajstić. Graph theory and Molecular Orbitals. Total φ-electron Energy of Alternant Hydrocarbons. *Chemical Physics Letters*, 17(4):535–538, 1972. doi:10.1016/0009-2614(72)85099-1.

[20] Haruo Hosoya. On some counting polynomials in chemistry. *Discrete Applied Mathematics*, 19(1-3):239–257, 1988. doi:10.1016/0166-218X(88)90017-0.

[21] Yeliz Kara, Yeşim Sağlam Özkan, Asad Ullah, Yasser Salah Hamed, and Melaku Berhe Belay. QSPR modeling of some COVID-19 drugs using neighborhood eccentricity-based topological indices: A comparative analysis. *PLoS One*, 20(5):e0321359, 2025. doi:10.1371/journal.pone.0321359.

[22] Louis H. Kauffman. A Tutte polynomial for signed graphs. *Discrete Applied Mathematics*, 25(1-2):105–127, 1989. URL: http://www2.math.uic.edu/~kauffman/TuttePolySignGraphs.pdf.

[23] V. R. Kulli. Different versions of Nirmala index of certain chemical structures. *International Journal of Mathematics Trends and Technology*, 67(3):50–57, 2021. doi:10.14445/22315373/IJMTT-V67I3P502.

[24] V. R. Kulli. Kepler Banhatti and Modified Kepler Banhatti Indices. *International Journal of Mathematics and Computer Research*, 12(6):4310–4314, 2024. doi:10.47191/ijmcr/v12i6.08.

[25] Virendra Kumar and Shibsankar Das. On Nirmala Indices-based Entropy Measures of Silicon Carbide Network. *Iranian Journal of Mathematical Chemistry*, 14(4):271–288, 2023. doi:10.22052/ijmc.2023.252742.1704.

[26] Virendra Kumar and Shibsankar Das. Comparative study between Nirmala and Sombor indices based on their applicability, degeneracy

and smoothness. *The European Physical Journal Plus*, 139:995, 2024. doi:10.1140/epjp/s13360-024-05768-x.

[27] Virendra Kumar and Shibsankar Das. QSPR Analysis of Thermodynamic Properties of Silicon Carbide Networks via Nirmala Indices-Based Entropy Measures. *Proceedings of the National Academy of Sciences, India Section A: Physical Sciences*, 2026. doi:10.1007/s40010-026-01071-9.

[28] Virendra Kumar, Shibsankar Das, and Jayjit Barman. Neighborhood degree sum-based entropy measures of some silicon carbide networks. *Journal of Chemical Sciences*, 137(4):123, 2025. doi:10.1007/s12039-025-02418-2.

[29] Young Chel Kwun, Mobeen Munir, Waqas Nazeer, Shazia Rafique, and Shin Min Kang. M-Polynomials and topological indices of V-Phenylenic Nanotubes and Nanotori. *Scientific Reports*, 7(1):8756, 2017. doi:10.1038/s41598-017-08309-y.

[30] Abid Mahboob, Ghulam Muhiuddin, Imran Siddique, and Sajid Mahboob Alam. A View of Banhatti and Revan Indices in Chemical Graphs. *Journal of Mathematics*, 2022:5680712, 2022. doi:10.1155/2022/5680712.

[31] Ante Miličević, Sonja Nikolić, and Nenad Trinajstić. On reformulated Zagreb indices. *Molecular Diversity*, 8:393–399, 2004. doi:10.1023/B:MODI.0000047504.14261.2a.

[32] Muhammad Nadeem, Sarfraz Ahmad, Muhammad Kamran Siddiqui, and Muhammad Naeem. Topological Descriptor of 2-Dimensional Silicon Carbons and Their Applications. *Open Chemistry*, 17(1):1473–1482, 2019. doi:10.1515/chem-2019-0155.

[33] H. M. Nagesh. Reverse Degree-Based Topological Indices and QSPR Analysis of Cancer Drugs, 2024. arXiv:2403.19686.

[34] Konstantin S. Novoselov, Andre K. Geim, Sergey V. Morozov, Da Jiang, Yang Zhang, Sergey V. Dubonos, Irina V. Grigorieva, and Anatoly A. Firsov. Electric field effect in atomically thin carbon films. *Science*, 306(5696):666–669, 2004. doi:10.1126/science.1102896.

[35] Milan Randić. Characterization of Molecular Branching. *Journal of the American Chemical Society*, 97(23):6609–6615, 1975. doi:10.1021/ja00856a001.

[36] Nenad Trinajstić, Douglas J. Klein, and Milan Randić. On some solved and unsolved problems of chemical graph theory. *International Journal of Quantum Chemistry*, 30(S20):699–742, 1986. doi:10.1002/qua.560300762.

[37] Damir Vukičević and Marija Gašperov. Bond Additive Modeling 1. Adriatic Indices. *Croatica Chemica Acta*, 83(3):243–260, 2010. URL: https://hrcak.srce.hr/en/62202.

[38] Heping Zhang and Fuji Zhang. The Clar covering polynomial of hexagonal systems I. *Discrete Applied Mathematics*, 69(1-2):147–167, 1996. doi:10.1016/0166-218X(95)00081-2.

[39] Dongming Zhao, Yu-Ming Chu, Muhammad Kamran Siddiqui, Kashif Ali, Muhammad Nasir, Muhammad Tayyab Younas, and Murat Cancan. On reverse degree based topological indices of polycyclic metal organic network. *Polycyclic Aromatic Compounds*, 42(7):4386–4403, 2022. doi:10.1080/10406638.2021.1891105.

[40] Dongming Zhao, Manzoor Ahmad Zahid, Rida Irfan, Misbah Arshad, Asfand Fahad, Zahid Ahmad, and Li Li. Banhatti, Revan and hyper-indices of silicon carbide $Si_2C_3 - \mathrm{III}[n, m]$. *Open Chemistry*, 19(1):646–652, 2021. doi:10.1515/chem-2020-0151.

© Scientific Annals of Computer Science 2026